COLLATZ BOUNDS AND THE COLLOCATION METHOD

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Technical Report No. 6

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Abstract

A systematic method is devised to obtain precise bounds in special eigenvalue problems. The method has the advantage that only differentiation is involved in the process once suitable trial functions are obtained. Compared with other bounding techniques in which extensive integrations are necessary, this method appears to have the advantage in simplicity. In application the method is ideally suited to the use of large-scale computers. Two illustrative problems are solved in order to demonstrate the capabilities of the technique.

Author

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Introduction

In many eigenvalue problems, the exact solution is very difficult to obtain and we must be content with approximate solutions. If the problem belongs to the class of special eigenvalue problems, it is well-known that Collatz bounds can be obtained very simply, but these bounds usually have such a wide spread that an accurate estimate of the exact result cannot be made. This paper suggests a method which enables a systematic improvement of the bounds with a minimum number of trial functions.

Theory

In an eigenvalue problem it is required to find one or more constants λ, generally called eigenvalues, and corresponding functions ψ, usually called eigenfunctions, such that a differential equation

$$M[\psi] = \lambda N[\psi] \tag{1}$$

is satisfied throughout a domain D subject to certain boundary conditions on the boundary of D. In general, the domain D may be either a one- or a two-dimensional continuum. For many eigenvalue problems M and N in Eq. (1) are both linear, homogeneous, self-adjoint, positive-definite, differential operators with the order of M greater than that of N. Under these conditions the eigenvalues are real and positive and the eigenfunctions form an orthogonal set.

When the eigenvalue does not appear in the boundary conditions, a continuous eigenvalue problem is called _special_ provided that the operator N has the form

$$N[\psi] = g\,\psi$$

where g is a prescribed continuous function which is positive throughout the domain D. Thus, the governing differential equation for special eigenvalue problems becomes

$$M[\psi] = \lambda\, g\, \psi \tag{2}$$

Many practical problems fall within the scope of the class of special eigenvalue problems. In particular we mention normal mode vibration problems. The development of this paper is applicable to special eigenvalue problems only.

Collatz[1] has devised an enclosure theorem applicable to special eigenvalue problems. In the formulation of the Collatz bounds a trial function v is selected such that the prescribed boundary conditions are identically satisfied. A function L is then defined in terms of v as follow:

$$L = \frac{M[v]}{g\ v} \tag{3}$$

If v is an eigenfunction ψ_i, then L defines a family of constants λ_i. If v is not an eigenfunction, then L varies throughout the domain D but the set of values taken by L possesses the following enclosure property:

> If L_{max} and L_{min} are the upper and lower bounds for L within the domain D, then there always exists at least one eigenvalue λ_i such that

$$L_{min} \leq \lambda_i \leq L_{max} \tag{4}$$

The separation of the bounds depends solely on the selection of the trial function v. If v is arbitrarily selected, the bounds will generally have such a wide separation that very little information on the exact eigenvalue λ is revealed. It is, therefore, highly desirable to develop a systematic procedure for improving the trial function v so that precise* bounds can be obtained.

The obvious way to accomplish this purpose is to select a trial function of the form

$$v = v_o + v_1 \tag{5}$$

where v_o and v_1 both satisfy the boundary conditions and are functionally independent of each other. Substituting this new trial function into Eq. (3) and otherwise following the same procedure will, in general, lead to somewhat better bounds. In principle, the bounds can be improved to any desired precision through the inclusion in v of additional independent trial functions v_i.

[1] L. Collatz, "Eigenvertaufgaben mit technischen Anwendung" Akademische Verlagsgesellschaft M. G. H., Leipzig (1949) p. 126

* The term "precise bounds" is herein used to infer that the separation of the bounds is small

In the meantime, the algebra becomes increasingly tedious.

Equation (5) can be generalized by inserting coefficients c_o and c_1 to obtain

$$v = c_o (v_o + a_1 v_1) ; \qquad a_1 = c_1/c_o \tag{6}$$

Upon substitution of the above expression into Eq. (3) we note that c_o cancels out. This is natural enough since, in eigenvalue problems, the mode shape is determinate to within a constant coefficient only. Henceforth, we set $c_o = 1$ without loss of generality. We now have

$$L = L(x,a_1)$$

Herein, we have used only a single spatial variable x but it should be understood that we can use two spatial variables if desired. By treating a_1 as a parameter, we can obtain an infinite family of bounds. From this family we can select the highest lower bound and the lowest upper bound which may not correspond to the same x and a_1; i.e.,

$$L_{min}\Big|_{\substack{x=x_1\\ a_1=k_1}} \leq \lambda \leq L_{max}\Big|_{\substack{x=x_2\\ a_1=k_2}} \tag{7}$$

These bounds are generally more precise than those obtained without using the parameter a_1.

To carry this procedure still further, we can let the trial function have the form

$$v = v_o + \sum_{p=1}^{P} a_p v_p \tag{8}$$

so that we have P parameters at our disposal. In principle, we can obtain the bounds by letting the a_p be any real numbers. This procedure is unwieldy and inefficient. In order to realize an improvement we require certain functional relations among the parameters a_p. Among the various methods available to achieve this goal, the collocation method is, perhaps, the simplest. In this method we require that the trial function v given by Eq. (8) satisfy Eq. (2) at P points in the domain D; i.e.,

$$\{ M \; [v] \; - \beta \, g \, v\}\Big|_{x=x_i} = 0, \quad (i=1,2,3,\ldots\ldots,P) \tag{9}$$

wherein we have replaced λ with β since satisfaction of Eq. (2) by v at discrete points $x=x_i$ does not yield the exact eigenvalue λ. Solving Eqs. (7) for a_p results in

$$a_p = a_p \; (\beta) \tag{10}$$

Now, all the coefficients a_p are related by a single parameter β and we obtain the following bounds:

$$L_{min}\Big|_{\substack{x=x_1 \\ \beta=\beta_1}} \leq \lambda \leq L_{max}\Big|_{\substack{x=x_2 \\ \beta=\beta_2}} \tag{11}$$

We observe that Eqs. (9) and (10) guarantee the satisfaction of Eq. (2) approximately in the sense that it is satisfied at P discrete points instead of at a generic point. We expect that the bounds obtained in this manner will be more precise than by other means presently available.

The Vibrating String

Perhaps the simplest of all normal mode vibration problems is that of the vibrating string. The exact eigenvalues are known to be $n^2\pi^2$, $n=1,2,\ldots$. We present the solution of this problem in order to demonstrate the merit of the method devised in the previous section. The governing differential equation in this case is

$$-\frac{d^2\psi}{d\,x^2} = \lambda\,\psi \qquad (12a)$$

subject to the following boundary conditions:

$$\psi\,(0) = \psi\,(1) = 0 \qquad (12b)$$

wherein the string is taken to be of unit length. Clearly, this is a special eigenvalue problem with

$$M\,[\ldots] = -\frac{d^2}{dx^2}\,[\ldots]$$

$$g = 1$$

Thus, we can calculate the Collatz bounds. First, we take

$$v = x - x^2$$

which satisfies the boundary conditions given by Eqs. (12b). Substitution into Eq. (3) results in

$$L = \frac{2}{x - x^2}$$

The denominator above must always be positive since $0 \leq x \leq 1$ so L approaches $+\infty$ as x approaches 0 or 1. Additionally, by symmetry, L has a stationary value, which must be a minimum, at $x = 1/2$. Thus, the largest and smallest values of L occur at $x=0$ and $x=1/2$ and, consequently, the Collatz bounds are

$$8 \leq \lambda \leq \infty$$

Let us now try

$$v = (x - x^2) + (x - x^2)^2$$

Substitution into Eq. (3) results in

$$L = \frac{12}{1 + x - x^2}$$

Now we observe that as x tends to zero, L approaches 12. Additionally, L has a minimum at $x = 1/2$ so that the largest and smallest values of L occur at $x = 0$ and $x = 1/2$, respectively. Thus, we get the following Collatz bounds in this case

$$9.6 \leq \lambda \leq 12$$

which is a substantial improvement over the previous case. We could continue in this fashion to obtain further improvement by adding additional terms to the trial function. Instead we will now make use of the method developed in the previous section.

Let us take the trial function v in the form given by Eq. (8) with

$$v_p = (x - x^2)^{p+1}, \quad (p = 0,1,2,\ldots) \tag{13a}$$

For one collocation point at $x_1 = 1/2$, P=1 and Eq. (9) becomes

$$\left(\frac{d^2 v}{d x^2} + \beta v \right) \Bigg|_{x=1/2} = 0 \tag{13b}$$

Substituting into this condition from Eq. (8) and using Eq. (13a) results in

$$a_1 = \frac{4 \ (\beta - 8)}{16 - \beta} \tag{13c}$$

Substitution into Eq, (3) from Eqs. (8) and (13c) results in

$$L = \frac{2 \ (48-5 \ \beta) + 48 \ (\beta-8)(x-x^2)}{(16-\beta)(x-x^2) + 4 \ (\beta-8)(x-x^2)^2} \tag{14a}$$

By appropriate limiting processes we obtain the following results:

$$\lim_{x \to 0} L = \begin{cases} + \infty, & 0 \leq \beta < 9.6 \\ + 12, & \beta = 9.6 \\ - \infty, & 9.6 < \beta \leq 16 \\ + \infty, & \beta > 16 \end{cases} \tag{14b}$$

In the event that $\beta = 9.6$, from Eq. (14a) we obtain

$$L = \frac{12}{1 + x - x^2}$$

We have seen this form of L before and we have the same bounds as previously derived; i.e.,

$$9.6 \leq \lambda \leq 12 \qquad (14c)$$

These are completely valid bounds but they are not necessarily the best bounds possible. We observe from Eq. (14b) that for every value of β except 9.6, L approaches $\pm\infty$ as x tends to zero. Thus, the other extrema of L must be stationary values of L. The conditions on the existence of stationary values of L are given by

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial \beta} = 0$$

Now, we differentiate Eq. (14a) with respect to x and set the result equal to zero to obtain

$$(1-2x)[(48-5\beta)(16-\beta) + 8(48-5\beta)(\beta-8)(x-x^2)+96(\beta-8)^2(x-x^2)^2]=0$$

The first term establishes the fact that there is a horizontal tangent to L at x=1/2 which must occur as a consequence of symmetry.

Thus, we obtain the following condition:

$$(48-5\ \beta)(16-\beta\ ) + 8(48-5\beta\ )(\beta-8)(x-x^2) + 96(\ \beta-8)^2(x-x)^2 = 0 \quad (15a)$$

Now we differentiate Eq. (14a) with respect to β and set the result equal to zero to obtain

$$x = \frac{1}{10}(5 \pm \sqrt{5}) \quad (15b)$$

which is valid for all β except $\beta = 48$ where $\partial L/\partial \beta$ is indeterminate. It is rather interesting to observe that this result is independent of β; i.e., regardless of the value of β(except for $\beta=48$), L is stationary with respect to β at the same spatial positions. Equation (15a) establishes the conditions under which L is stationary with respect to x while Eq. (15b) establishes the spatial position of the stationary value of L with respect to β. If both of these conditions are satisfied simultaneously, we obtain the values of β and x for which L is stationary with respect to both variables simultaneously. Substitution from Eq. (15b) into Eq. (15a) yields

$$\beta = 9.905$$

Substitution from Eq. (15b) into Eq. (14a) obtains

$$L = 10$$

We see that every L-curve of the family must have a value of 10 at $x = (5 \pm \sqrt{5})/10$ but only when $\beta = 9.905$ is L stationary. From Eq. (14b) we see that for $9.6 < \beta \leq 16$, L tends to $-\infty$ as x approaches 0 or 1. Thus, the stationary value of L at $x = (5 \pm \sqrt{5})/10$ for $\beta = 9.905$ must be a maximum and, consequently, we obtain the following bounds on the eigenvalue

$$-\infty \leq \lambda \leq 10 \tag{16}$$

From Eqs. (14c) and (16) we finally obtain the following bounds on the fundamental eigenvalue

$$9.6 \leq \lambda \leq 10$$

We have achieved a modest inprovement in the bounds over those obtained with the previous trial function.

In order to improve these bounds we proceed to a two-point collocation solution. As collocation points we select $x = 0$ and 1/2. Now, the trial function is given by

$$v = (x - x^2) + a_1 (x - x^2)^2 + a_2 (x - x^2)^3 \tag{17a}$$

The collocation conditions are given by

$$\left(\frac{d^2v}{dx^2} + \beta v\right)\bigg|_{x=o} = \left(\frac{d^2v}{dx^2} + \beta v\right)\bigg|_{x=1/2} = 0 \tag{17b}$$

Substitution into these conditions from Eq. (17a) results in two algebraic equations which we readily solve to get

$$a_1 = 1, \qquad a_2 = \frac{4\,(48 - 5\,\beta)}{\beta - 24} \tag{17c}$$

Substituting from Eq. (17a) into Eq. (3) and using Eqs. (17c) leads to

$$L = \frac{12\,[\,(11\beta - 120) + 10\,(48-5\beta)\,(x-x^2)\,]}{(\beta-24)\,(1+x-x^2) + 4(48-5\beta)\,(x-x^2)} \tag{17d}$$

We must now find the extrema of L with respect to x and β. We can use the customary methods of finding extrema, as we have previously done; however, now the algebra involved becomes excessively complicated and tedious. A more profitable approach is to make use of a computer at this point. The general idea of the computer program is to calculate L_{min} and L_{max} corresponding to a given β. We are led, in the selection of β, by the fact that, as the separation of the bounds on the eigenvalue λ becomes smaller, β will approach λ. Thus, the value of β that will yield the best bounds will lie in the range

$$9.6 \leq \beta \leq 10.0$$

The procedure is to select several values of β in this range and, corresponding to each value of β we calculate bounds on λ by means of the computer program. Finally, from among these bounds we select the highest lower bound and the lowest upper bound. These two bounds will ordinarily correspond to two different values of β. Following this procedure for the two-point collocation solution defined by Eqs. (17) we obtained the following bounds:

$$9.85 \leq \lambda \leq 9.87$$

We see that the total separation of the bounds is only 0.2 per cent. This would also correspond to the maximum error in the eigenvalue.

We can obtain still more improvement by proceeding to a three-point collocation solution. Using the collocation points $x = 0$, $1/4$ and $1/2$, we obtained the following bounds:

$$9.869 \leq \lambda_1 \leq 9.870$$

where the maximum error is only 0.01 per cent. This is probably more accurate than is usually required but the calculation was carried out to demonstrate the possibilities of the method proposed herein. The procedure is very straight-forward and the computer programs involved, while not trivial, are extremely simple. Let us now proceed to a somewhat more complicated illustrative example.

Axial-Shear Vibrations of a Long Bar

The axial-shear mode of free vibrations is that mode wherein the only non-zero component of displacement is the axial component and it was shown by Baltrukonis and Gottenberg[2] that the governing differential equation is

$$\nabla^2 \psi = \frac{\rho}{G} \frac{\partial^2 \psi}{\partial t^2} \tag{18a}$$

wherein ∇^2 denotes the usual Laplacian differential operator, ψ denotes the axial component of displacement in this case, ρ and G denote the mass density and shear modulus of the bar material while t denotes time. Since we are interested in free, harmonic oscillations, we define

$$\psi = \Psi e^{i\omega t} \tag{18b}$$

and, consequently, from Eq. (18a) we obtain

$$-\nabla^2 \Psi = \lambda \Psi \tag{18c}$$

wherein

$$\lambda = \rho\omega^2/G \tag{18d}$$

[2] Baltrukonis, J. H. and W. G. Gottenberg "Thickness-Shear Vibrations of Circular Bars" J. Acoust. Soc. Amer. 31 734 (June 1959)

If the shape of the cross-section of the bar is natural to any common coordinate system, we can use Eq. (18c) directly to obtain bounds on the fundamental natural frequency of free vibrations in the mode under consideration. However, if the bar has a particularly complicated cross-section, it may be very difficult to obtain a system of trial functions which satisfy the boundary conditions identically. To alleviate this difficulty, we can transform the domain onto a simpler region by mean of a mapping function of the form

$$z = z(\xi)$$

The governing differential equation is transformed into

$$-\nabla^2 \Psi = \lambda \left| \frac{dz}{d\xi} \right|^2 \Psi \tag{19}$$

in the transformed region. Note that this problem remains a special eigenvalue problem since

$$\left| \frac{dz}{d\xi} \right|^2 > 0$$

We shall treat the problem of a long, prismatical bar with an epitrochoidal cross-section which is clamped such that the displacements along the lateral surfaces of the bar vanish identically. This cross-section is transformed onto a circular region by means of the following mapping function

$$z = R\,\xi(1 + m\,\xi^{n}) \tag{20}$$

where n denotes the number of axes of symmetry of the region while m is a shape factor. In the present illustrative problem we let n = 4 and m = 1/6. The governing differential equation in the unit circular region in the ξ - plane is given by

$$-\left(\frac{\partial^2\Psi}{\partial r^2}+\frac{1}{r}\frac{\partial\Psi}{\partial r}+\frac{1}{r^2}\frac{\partial^2\Psi}{\partial\theta^2}\right)=\lambda\left(1+\frac{5}{3}r^4\cos 4\theta+\frac{25r^8}{36}\right)\Psi \tag{21}$$

We now define the function L as follows:

$$L=-\left[\left(1+\frac{5}{3}r^4\cos 4\theta+\frac{25}{36}r^8\right)v\right]^{-1}\left(\frac{\partial^2 v}{\partial r^2}+\frac{1}{r}\frac{\partial v}{\partial r}+\frac{1}{r^2}\frac{\partial v^2}{\partial\theta^2}\right) \tag{22}$$

wherein v denotes an approximation to the exact eigenfunction Ψ which must, of course, identically satisfy the boundary conditions on Ψ. As a system of trial functions we take

$$v_p = (1 - r^2)^{p+1}, \quad p = 0,1,2,\ldots\ldots\ldots,P \tag{23a}$$

Let us calculate the bounds for the simplest case P=0. Then,

$$v = v_o = 1 - r^2 \tag{23b}$$

Substituting into Eq. (22) and searching for the largest and smallest values of L results in the following Collatz bounds

$$4 \leq \lambda_1 \leq + \infty$$

These are poor bounds, indeed, but another improved set can be readily obtained by introducing a new system of trial functions u_p (p=0,1,2,.....,P) which identically satisfy the boundary conditions on the exact eigenfunction and are related to v_p by

$$M\ [u] = N\ [v] \tag{24a}$$

In this particular case we have

$$-\left(\frac{\partial^2 U}{\partial r^2} + \frac{1}{r}\frac{\partial U}{\partial r} + \frac{1}{r^2}\frac{\partial^2 U}{\partial \theta^2}\right) = \left(1 + \frac{5}{3} r^4 \cos 4\theta + \frac{25}{36} r^8\right) V \tag{24b}$$

Corresponding to v_o, as given by Eq. (23b), we find

$$U_0 = \frac{1}{4}(1-r^2) - \frac{1}{16}(1-r^4) + \frac{1}{144}(1-r^{10}) - \frac{25}{5184}(1-r^{12}) + \left[\frac{1}{12}r^4(1-r^2) - \frac{5}{144}r^4(1-r^4)\right]\cos 4\theta \tag{24c}$$

We calculate L from Eq. (22) by replacing v with u. Using Eq. (24c) then results in

$$L = (1 - r^2)/u_0 \tag{24d}$$

Thus, we readily find the following Collatz bounds

$$5.3 \leq \lambda_1 \leq 8.6$$

Which represent a considerable improvement over the previous bounds. Nonetheless, in many applications much greater precision is required and we proceed to apply the method proposed in the present paper.

As before, we define

$$v = v_0 + a_1 v_1 \tag{25a}$$

wherein

$$v_0 = 1 - r^2 \tag{25b}$$

$$v_1 = (1 - r^2)^2 \tag{25c}$$

Using Eq. (24a) we calculate

$$u = u_o + a_1 u_1 \tag{26}$$

We then obtain a_1 by collocation at the generic point (r_1, θ_1). The following collocation condition is obtained from Eq. (21):

$$\left[\left(\frac{\partial^2 U}{\partial r^2} + \frac{1}{r}\frac{\partial U}{\partial r} + \frac{1}{r^2}\frac{\partial^2 U}{\partial \theta^2}\right) + \beta\left(1 + \frac{5}{3} r^4 \cos 4\theta + \frac{25}{36} r^8\right) U\right]\Bigg|_{\substack{r=r_1\\ \theta=\theta_1}} = 0 \tag{27a}$$

wherein we have used β rather than λ since u is only an approximation to the eigenfunction. Using Eq. (24a), we can rewrite this collocation condition as follows:

$$\left(1 + \frac{5}{3} r^4 \cos 4\theta + \frac{25}{36} r^8\right)\left(V - \beta U\right)\Bigg|_{\substack{r=r_1\\ \theta=\theta_1}} = 0$$

The first factor does not, in general, vanish and, therefore, we finally obtain the following collocation condition:

$$(v - \beta u)\Bigg|_{\substack{r=r_1\\ \theta=\theta_1}} = 0 \tag{27b}$$

Substitution from Eqs. (25a) and (26) yields

$$a_1 = - \left. \frac{V_0 - \beta U_0}{V_1 - \beta U_1} \right|_{\substack{r=r_1 \\ \theta=\theta_1}} \tag{27c}$$

If, in Eq. (22), we replace v with u and use Eq. (24a), we obtain

$$L = - \frac{v_0 + a_1 v_1}{u_0 + a_1 u_1} \tag{28}$$

Once again we select a series of values for β. Corresponding to each value of β we calculate a set of bounds on the eigenvalue λ_1 by using Eq. (28). From among these sets of bounds we selected the lowest upper bound and the highest lower bound to finally obtain

$$5.56 \leq \lambda_1 \leq 5.80$$

We could continue in the same manner to obtain even more accurate bounds.

Using the much more complicated Kohn-Kato enclosure theorem, Baltrukonis, Chi, and Laura[3] calculated the following bounds on the eigenvalue in this problem

$$5.682 \leq \lambda_1 \leq 5.689$$

The bounds obtained by the much simpler method proposed herein compare very favorably.

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[3] Baltrukonis, J. H., M. Chi and P. Laura "Axial-Shear Vibrations of Star-Shaped Bars - Kohn-Kato Bounds", <u>Developments in Mechanics</u>, Pergamon Press (1964)